Lyapunov exponent and transfer-matrix spectrum of the random binary alloy

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The one-dimensional Anderson model with binary distributed onsite disorder is investigated using the transfer-matrix approach. The random matrix product is transformed into an iterated conformal map and the convergence of the mapping is studied for various values of the concentration of onsite impurities and the energy. For dilute impurity concentrations the convergence of the mapping is strongly energy dependent and exhibits interesting behavior in the complex mapping plane. As the impurity concentration increases the mapping converges to the unit circle which results from the underlying conformal structure. Explicit expressions for the Lyapunov exponent and the eigenvalues of the transfer matrix are obtained in terms of the conformal map. From the Lyapunov exponent, the localization length and the integrated density of states are calculated. In the dilute limit there exist states in which the localization length exceeds the system size. These states correspond to extended electronic states and it is shown that the number of extended states scales with system size as $N_{\text{extended}} \propto N^{-2}$. Increasing the impurity concentration beyond a critical value destroys these states and the localization length over the entire energy range becomes smaller than the system size.

I. INTRODUCTION

Products of random 2×2 matrices often occur in the study of disordered one-dimensional systems. The simplest example of a disordered one-dimensional electronic system is the random binary alloy (RBA), a one-dimensional Anderson model with binary distributed onsite disorder.[1,2] Despite the apparent simplicity of the one-dimensional Anderson model many interesting results have been obtained. It can be proved that in one dimension, arbitrarily small amounts of disorder lead to exponentially localized electronic states provided the distribution of disorder satisfies certain ergodic requirements.[1,3,4] Furthermore, it has been shown that extended electronic states can exist if the distribution of the disorder is correlated. The existence of extended states has been observed in the random dimer model and originates from perfect transmission through the dimer defect for a select set of energies.[5–7] This result is consistent with the restrictions placed on the ergodic requirements for the distribution of the disorder[4] and has interesting consequences with regard to transport properties.[5–7] Recent theoretical work has demonstrated the existence of extended electronic states for the Thue-Morse aperiodic lattice. This new type of correlated disorder does not depend on perfect transmission through a single dimer defect.[8,9]

A physical realization of the one-dimensional disordered electronic system is the disordered polymer chain. Recent theoretical studies of doped polyacetylene have been performed for diagonal and off-diagonal disorder within a disordered tight-binding model including electron-phonon interactions (Su-Schrieffer-Heeger model).[10–12] Furthermore, the random dimer model with correlated disorder has also been proposed as a model of doped polyaniline and various transport properties have been calculated.[5] As previously stated, this model has extended states and has been used to explain the insulator-metal transition observed in doped polyaniline. The RBA can be envisioned as a model for a disordered conjugated polymer with conformational disorder. The conformational disorder arises due to random breaks in conjugation, and is modeled by the onsite energy barrier to hopping. It has also been proposed as a model for the electronic structure of proteins.[13]

Many theoretical techniques have been applied to the study of one-dimensional disordered electronic systems. Direct calculations employing Green's functions have been widely used and have been applied to the one-dimensional Anderson model.[14,15] This technique gives the localization length and density of states from the real and imaginary parts of the averaged Green's function and can also be used to calculate transport related averages.[14,15] Alternatively, the transfer-matrix approach allows for the calculation of the Lyapunov exponent of the random matrix product. From the Lyapunov exponent, the localization length and density of states can be determined from the real and imaginary parts of the Lyapunov exponent through the Thouless formula.[1,2] The analytic calculation of the Lyapunov exponent is quite difficult and perturbative expansions for the Lyapunov exponent for the one-dimensional Anderson model have been developed.[16,17] This type of weak disorder expansion is valid in the limit of vanishing disorder, and for the one-dimensional Anderson model gives rise to nonanalytic behavior for the Lyapunov exponent near the band edge in the weak disorder limit.[16] Recently, a technique based on the transformation of the random matrix product to an iterated conformal map has been used to study the analytic properties of the random bond Ising model and a formal expression for the Lyapunov exponent for the spin glass has been obtained.[18]

In the present work, the RBA is formulated as a random matrix product using the transfer-matrix technique.

The 2×2 transfer matrices are transformed into a complex matrix representation by a site-independent rotation. The complex representation of the transfer matrices induces a Möbius transformation on the extended complex plane.[18] The random 2×2 matrix product can therefore be expressed as an iterated conformal mapping. This technique allows for the underlying analytic structure of the random matrix product to appear as a natural consequence of the conformal mapping of the extended complex plane. The iteration of the conformal map leads to various types of convergence properties in the complex mapping plane as a function of the onsite impurity concentrations and the electronic energy. The convergence properties of the mapping and its analytic structure are examined.

Explicit expressions for the Lyapunov exponent and the eigenvalues of the random matrix product are obtained in terms of the conformal map. From the Lyapunov exponent, the localization length and the integrated density of states (IDOS) are calculated as a function of energy for various values of onsite impurity concentrations. The dilute impurity case shows extended electronic states on a finite lattice but investigation of the scaling behavior with system size indicates that the extended states do not survive the continuum limit. From the convergence of the mapping, approximate expressions for the Lyapunov exponent are obtained which are valid in the continuum limit.

II. RANDOM BINARY ALLOY

The equation of motion for the one-dimensional Anderson model with binary onsite disorder (RBA) is given by

$$(E-\epsilon_n)c_n = V(c_{n+1}+c_{n-1}), \tag{1}$$

where $V<0$ is the nearest-neighbor hopping integral, and c_n is the probability amplitude on the nth site. The random onsite energy $\epsilon_n = (\epsilon_a, \epsilon_b)$ takes two values with probability p and $1-p$, respectively. In the absence of disorder, the system is translationally invariant and the energy dispersion relation is given by $E = 2V\cos(ka)$, where a is the lattice constant. From the energy expression it is clear that at the Brillioun zone boundary, $k = \pm\pi/a$, the density of states has a square root singularity at $E = 2|V|$. The effect of disorder is seen to shift the density of states and to smooth the square root singularity.

The tight-binding equation of motion for the disordered chain can be readily formulated using transfer matrices. The transfer matrix is defined by

$$x_{n+1} = T_n x_n, \tag{2}$$

where

$$T_n = \begin{pmatrix} \frac{E-\epsilon_n}{V} & -1 \\ 1 & 0 \end{pmatrix}, \tag{3}$$

which are treated as independent random matrices, and

$$x_n = \begin{pmatrix} c_n \\ c_{n-1} \end{pmatrix}. \tag{4}$$

The random matrix product is obtained by iterating Eq. (2) to give, $x_{n+1} = T_n T_{n-1}\cdots T_2 T_1 x_1$, where x_1 is an initial vector of coefficients.

It is convenient to perform a site-independent rotation of the transfer matrices to obtain a complex representation of the transfer matrices. The transformation leaves the trace of the product and the norm of the x's invariant. The rotated transfer matrices are of the form, $t_n = U^\dagger T_n U$, where U is a Hermitian matrix given by

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ -i & -1 \end{pmatrix}. \tag{5}$$

Explicitly, we obtain

$$t_n = \left(\frac{E-\epsilon_n}{2V}\right)\begin{pmatrix} z_n & i \\ -i\,\bar{z}_n & \end{pmatrix}, \tag{6}$$

where

$$z_n = 1 + i\frac{2V}{(E-\epsilon_n)}. \tag{7}$$

It has been demonstrated previously that complex transfer matrices of the form given in Eq. (6) induce a Möbius transformation of the extended complex plane. The conformal group structure enables a simple representation for the matrix product as an iterated conformal map.[18]

III. LYAPUNOV EXPONENT AND CONFORMAL MAPPING

The Lyapunov exponent gives the exponential rate of growth of the random matrix product and is defined as

$$\gamma(E) = \lim_{n\to\infty} \frac{\ln(\|T_n T_{n-1}\cdots T_2 T_1 x_1\|)}{n\|x_1\|}, \tag{8}$$

where $\|\ \|$ is the vector norm. At first sight, the Lyapunov exponent seems to depend on the norm of the initial vector ($\|x_1\|$), but it can be shown that for almost any realization of the disorder, the maximal Lyapunov exponent exists with unit probability[19] and is given by

$$\gamma(E) = \lim_{n\to\infty}\frac{1}{n}\ln\left[\mathrm{Tr}\left(\prod_{k=1}^{n} T_k\right)\right]. \tag{9}$$

Therefore, the quantity of interest is the trace of the product of the transfer matrices. It has been previously shown that the trace of a product of noncommuting matrices of the form derived in Eq. (6) can be written as[18]

$$\mathrm{Tr}\left(\prod_{n=1}^{N} T_n\right) = \Lambda_N^{(+)}(E) + \Lambda_N^{(-)}(E), \tag{10}$$

where $\Lambda_N^{(\pm)}(E)$ are conjugate. Here $\Lambda_N^{(+)}(E)$ is defined as

$$\Lambda_N^{(+)}(E) = \prod_{n=1}^{N}\left(\frac{E-\epsilon_n}{2V}\right)(r_n + z_n), \tag{11}$$

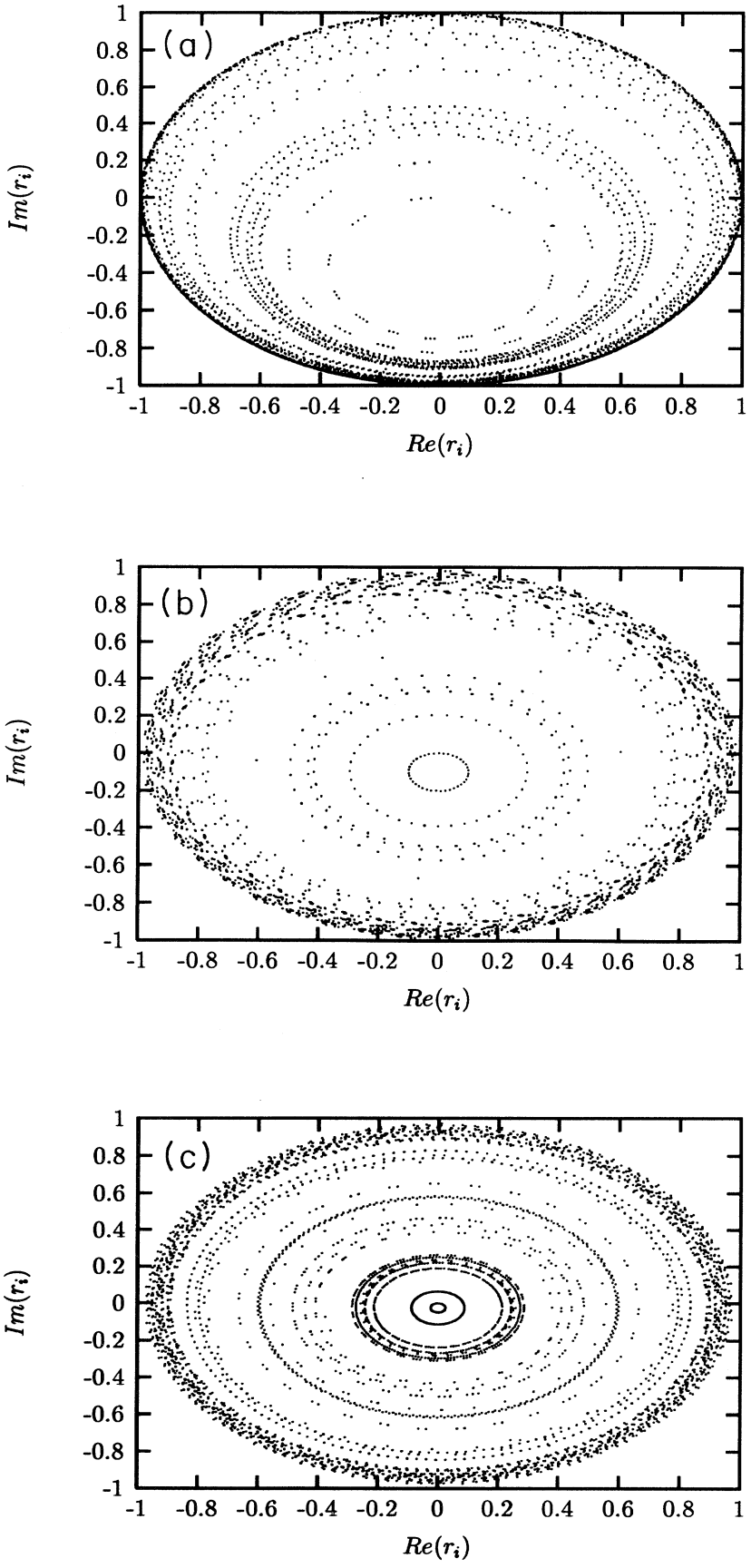

FIG. 1. Plots of the $\mathrm{Im}(r_i)$ versus $\mathrm{Re}(r_i)$ for various energy values: (a) $E = -1.0$, (b) $E = 0.1$, (c) $E = 0.4$, where $N = 14\,000$, $V = -1.0$ and the impurity concentration is $p = 0.01$.

where the conformal map variable r_n is given by

$$r_{n+1} = \frac{1 + \bar{z}_n r_n}{r_n + z_n}, \tag{12}$$

with the initial condition $r_1 = 0$. The iterated conformal map in Eq. (12) is of the form of a Möbius transformation of the extended complex plane. It has the property that it maps circles into circles in the complex plane. Moreover, it maps the unit circle onto the unit circle and it's these properties of the mapping that will prove very important when the random binary alloy is examined.

The random binary alloy can now be considered and the convergence properties of the map examined for the specific case of onsite energies $\epsilon_a = 0.5$ and $\epsilon_b = 0.0$ chosen with probability p and $1 - p$, respectively. Here p represents the concentration of onsite impurities. In Fig. 1, we show the convergence in the complex mapping plane for various values of energy in the range $-2|V| + \epsilon \leq E \leq 2|V|$ with onsite impurity concentration fixed at $p = 0.01$. We find an interesting pattern of concentric circles in the complex plane. These concentric circles are centered on the imaginary axis at $(E - \epsilon_a)/4|V|$ and pass through the origin, which is due to the initial condition of the map. The radius of the circles increase with iteration eventually intercepting the unit circle where the map subsequently remains. This results from the invariance of the unit circle under the action of the Möbius transformation. As the impurity concentration is increased, the pattern is destroyed, as seen in Fig. 2 where $p = 0.1$. The map converges rapidly to the complete unit circle for energies in the range $-2|V| + \epsilon \leq E \leq 2|V|$. Further increase of the onsite impurity concentration gives rise to rapid convergence to the unit circle and will provide the basis for an approximation scheme for the Lyapunov exponent.

The Lyapunov exponent for the random binary alloy on a finite lattice of N sites can be obtained from the general definition in Eq. (9) and is given by

$$\gamma_N(E) = \frac{\ln[\Lambda_N^{(+)}(E)]}{N}, \tag{13}$$

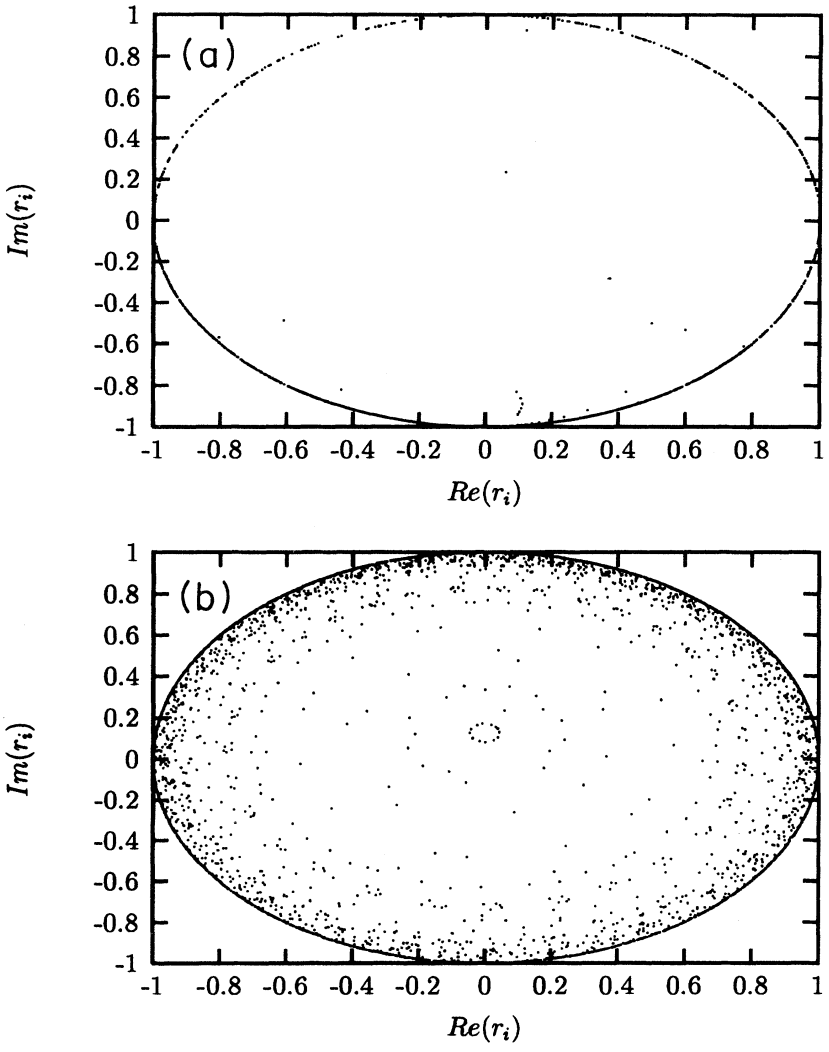

FIG. 2. Plots of the $\mathrm{Im}(r_i)$ versus $\mathrm{Re}(r_i)$ for various energy values: (a) $E = -1.5$, (b) $E = 1.0$, where $N = 14\,000$, $V = -1.0$, and the impurity concentration is $p = 0.1$.

which is a complex-valued quantity. From the Thouless formula, the localization length $\zeta_N(E)$ is defined by

$$\mathrm{Re}[\gamma_N(E)] = 1/\zeta_N(E), \tag{14}$$

and the integrated density of states (IDOS) is defined by

$$\mathrm{Im}[\gamma_N(E)] = \int^E \rho_N(\omega)d\omega. \tag{15}$$

In Fig. 3, the localization length and the IDOS are computed for the various concentrations of onsite impurities used in Figs. 1 and 2. For the dilute case $p = 0.01$ shown in Fig. 3(a), we find that for a discrete set of energy values, there exist localization lengths which are greater than the size of the system. This implies the existence of extended states since the localization length determines the exponential envelope of the electronic wave function. In Fig. 3(b), we find that the extended states disappear as the concentration of impurities is increased and the convergence of the map to the unit circle is rapid. For all values of impurity concentration greater than some critical impurity concentration p_c, we find that all states are exponentially localized for a fixed system size N. Furthermore, the extended states for the dilute case are robust under differing realizations of the disorder but depend quite crucially on the number of sites. Thus, one must investigate how the number of extended states N_{extended} scales with the system size N to determine if extended states survive the continuum limit.

In Fig. 4, the number of extended states (i.e., states with localization length greater than the system size) is plotted versus the system size N on a log-log scale. The line is a fit to $N_{\mathrm{extended}} = AN^{-2}$. From the scaling behavior it is clear that the number of extended states in the continuum limit is zero for the random binary alloy. However, the existence of extended electronic states will influence the transport properties of the finite chain and may be realized in conformationally disordered conjugated polymers. These polymers consist of long but finite chain backbones which have random breaks in conjugation. This type of disorder is intrinsic and is not necessarily a result of the action of an external source such as doping.

In Figs. 3(a) and 3(b), the IDOS is computed. The IDOS rises rapidly at $E = -2|V| + \epsilon_a$ and increases smoothly in the energy range $-2|V| + \epsilon \leq E \leq 2|V|$.

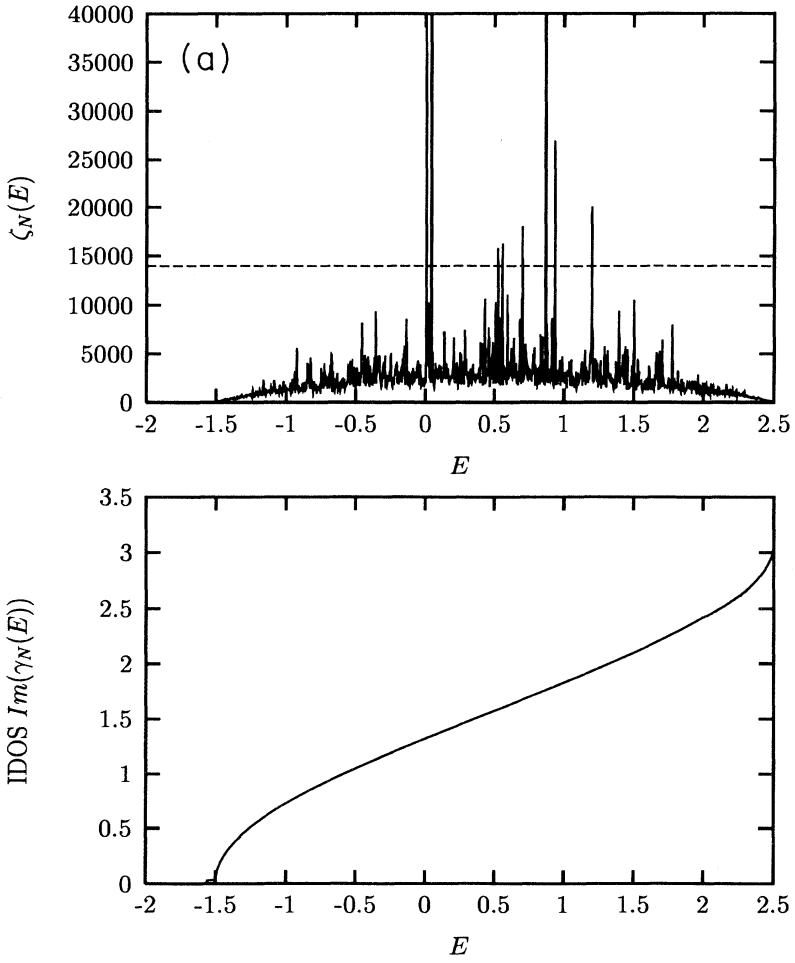

FIG. 3. (a) The localization length (top) and the integrated density of states (bottom) for $p = 0.01$. (b) The localization length (top) and the integrated density of states (bottom) for $p = 0.1$.

At the upper band edge $E = 2|V|$, there is a cusp in the IDOS for the case $p = 0.1$ which results from the smoothed square root singularity in the density of states. For the dilute case $p = 0.01$, the cusp in the IDOS is not present and the IDOS appears shifted by the onsite energy $\epsilon_a = 0.5$.

From the convergence of the map shown in Figs. 1 and 2, it should be noted that for all but the dilute case, the mapping converges rapidly to the unit circle. The points are dense on the unit circle as can be seen from the underlying Möbius transformation. It is therefore convenient to approximate the map variable by $r_n \approx e^{i\theta_n + i\delta_n}$ where $\theta_n = \tan^{-1}[2V/(E - \epsilon_n)]$. Therefore, the approximate Lyapunov exponent is given by

$$\gamma_N(E) = \frac{1}{N}\sum_{n=1}^{N} \ln\left|\frac{E-\epsilon_n}{2V}\right| + i\left[\pi\Theta\left(\frac{\epsilon_n - E}{2V}\right) + \tan^{-1}\left(\frac{2V}{E-\epsilon_n}\right)\right] + \ln\left(e^{i\delta_n} + |z_n|\right), \tag{16}$$

where Θ is a Heaviside step function. The approximate phase of the mapping δ_n can be obtained (see the Appendix) and is given by $\delta_{n+1} = \delta_n - (\theta_{n+1} + \theta_n)$, where the initial phase is arbitrary since the resulting expression is valid after the map has converged to the unit circle.

In Figs. 5(a) and 5(b), we plot the approximate expression for the localization length and IDOS. It can be seen that the agreement for the magnitude of the localization

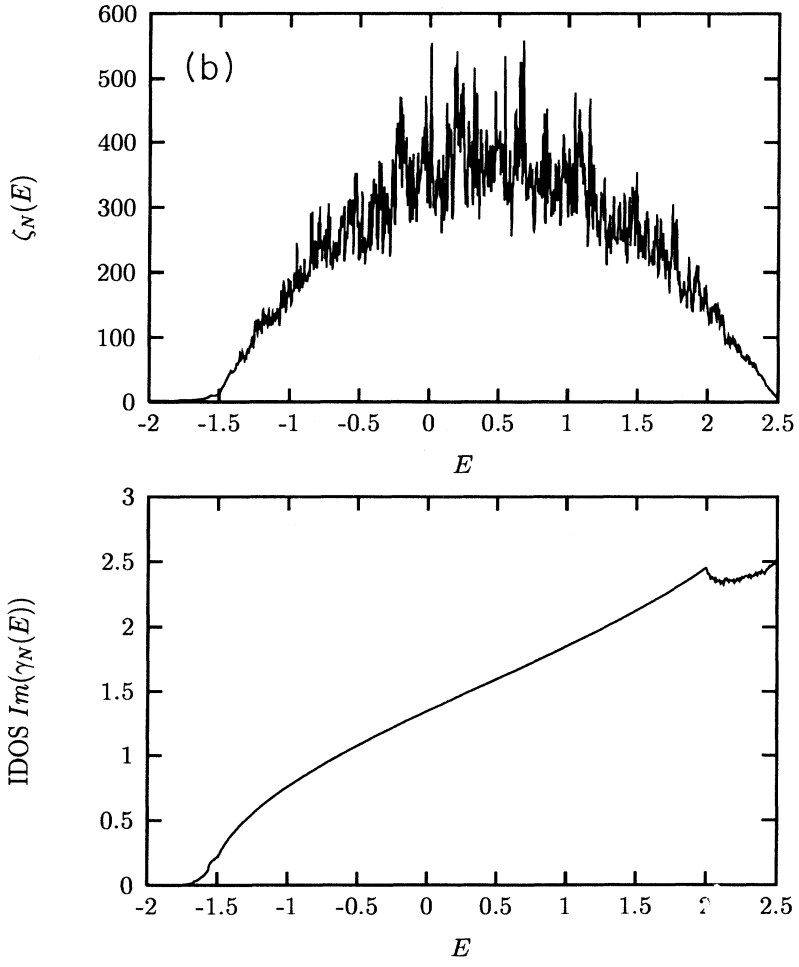

FIG. 3 *(Continued).*

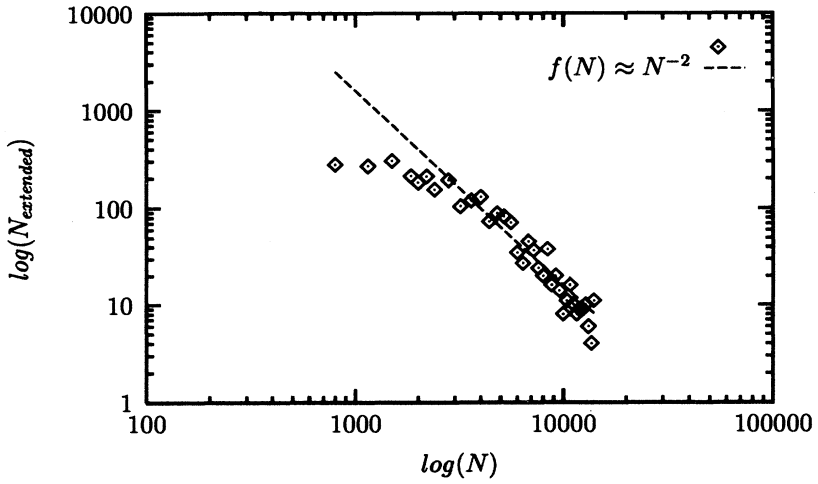

FIG. 4. Log-log plot of the number of extended states versus the system size for $p = 0.01$ [i.e., $\log(N_{\text{extended}})$ versus $\log(N)$]. The line is a fit to $N_{\text{extended}} \propto N^{-2}$.

length is quite good but the width in energy is much too narrow. It is also important to note that the most extended electronic states are centered on the onsite energy $E = 0.5$. We also find that the approximated IDOS is a smooth function of energy and deviates from the exact calculated IDOS near the band edge, $E \approx -2|V| + 0.5$ and $E \approx 2|V|$. See Figs. 3(a) and 3(b) for a comparison. The approximate density of states can be obtained by differentiating the imaginary part of the approximate Lyapunov exponent (IDOS) given in Eq. (16). The expression derived in Eq. (16) is valid in the continuum limit since it is expected that the map converges to the

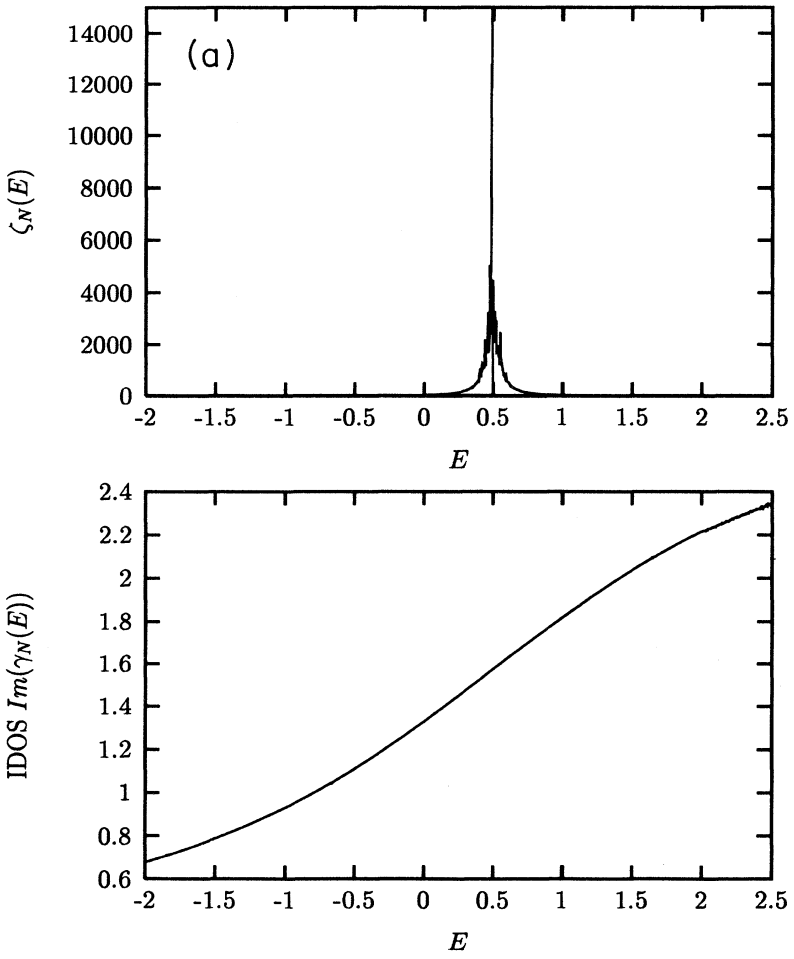

FIG. 5. (a) The approximate localization length (top) and the integrated density of states (bottom) for $p = 0.01$ [see Fig. (3a) for comparison]. (b) The approximate localization length (top) and the integrated density of states (bottom) for $p = 0.1$ [see Fig. 3(b) for comparison].

unit circle after a finite number of iterations. From the approximate result for the dilute case it is seen that extended states do not exist for $E \neq \epsilon_a$ in the continuum limit in agreement with the scaling result

From the calculation of the Lyapunov exponent, we turn our attention to the eigenvalues of the transfer-matrix product. The eigenvalues can be determined using the trace and determinant formula. In general, we define $M_N = \prod_{n=1}^{N} T_n$. It is known that $\mathrm{Tr}(M_N) = \lambda_+ + \lambda_-$ and $\det(M_N) = \lambda_+ \lambda_-$. It is therefore a simple matter to solve for the eigenvalues of the transfer matrix product using $\mathrm{Tr}(M_N)$ and

$$\lambda_+ - \lambda_- = \sqrt{[\mathrm{Tr}(M_N)]^2 - 4\det(M_N)}.$$

We therefore obtain

$$\lambda_\pm = \frac{1}{2}\{\mathrm{Tr}(M_N) \pm \sqrt{[\mathrm{Tr}(M_N)]^2 - 4\det(M_N)}\}. \quad (17)$$

The two eigenvalues of the transfer-matrix product in terms of the conformal mapping parameters are given by

$$\lambda_\pm(E) = \prod_{n=1}^{N}\left(\frac{E-\epsilon_n}{2V}\right)\left[\prod_{n=1}^{N}(r_n + z_n) + \prod_{n=1}^{N}(\bar{r}_n + \bar{z}_n) \pm \sqrt{\left(\prod_{n=1}^{N}(r_n + z_n) + \prod_{n=1}^{N}(\bar{r}_n + \bar{z}_n)\right)^2 - 4\prod_{n=1}^{N}(|z_n|^2 - 1)}\right]. \quad (18)$$

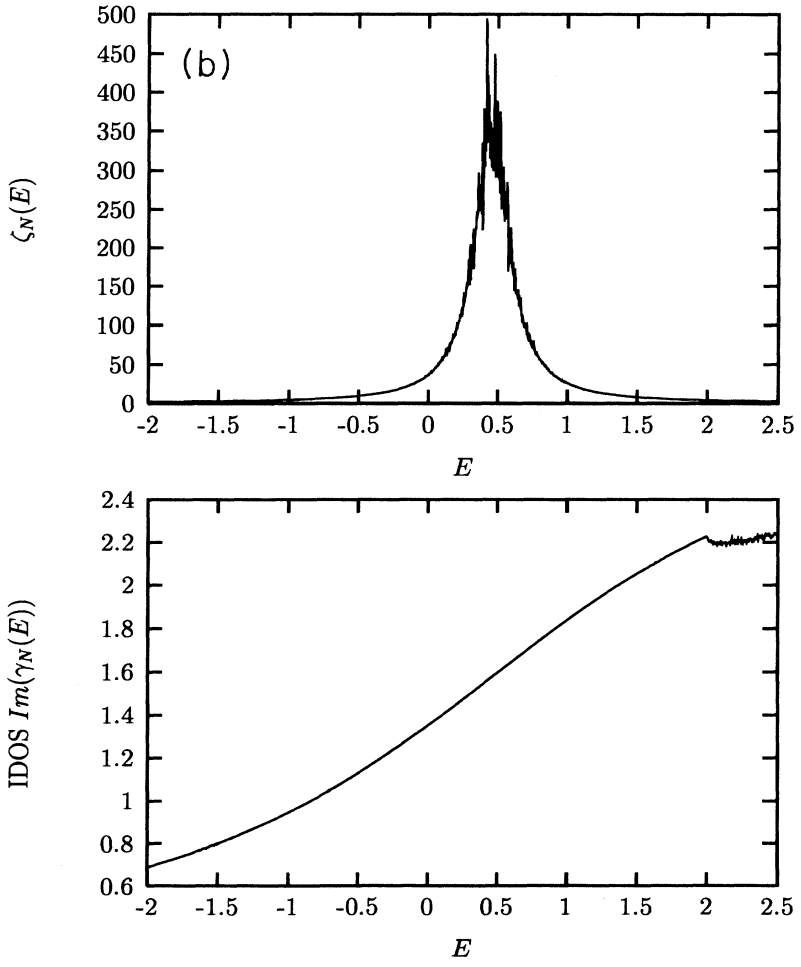

FIG. 5 *(Continued).*

Therefore, the convergence properties of the map directly determine the spectral properties of the transfer-matrix product, and we have completely characterized the random matrix product.

IV. CONCLUSIONS

We have shown that the random binary alloy can be expressed as a product of random matrices. The random matrix product can be transformed to an iterated conformal map and the convergence properties in the complex mapping plane examined.

The convergence of the iterated conformal mapping has been studied as a function of energy and disorder. The convergence properties result from the underlying Möbius transformation and the convergence to the unit circle for energies in the range $-2|V|+\epsilon \leq E \leq 2|V|$ has been demonstrated for all densities of onsite impurities. For the most dilute cases, we find interesting patterns of concentric circles generated in the complex mapping plane which ultimately converge to the unit circle.

Furthermore, explicit expressions for the Lyapunov exponent and the eigenvalues of the transfer-matrix product are obtained in terms of the conformal map from which the localization length and the integrated density of states are computed. It is found that for dilute concentrations of onsite defects on finite lattices there exist extended electronic states for energies not equal to the onsite energy. These states scale approximately as the inverse square of the number of sites and thus do not contribute in the continuum limit. These extended electronic states may exist in finite disorder lattices such as conformationally disordered polymers and affect the electronic transport properties.

From the convergence properties of the mapping, approximate expressions for the Lyapunov exponent and the eigenvalues can be obtained. These expressions will be approximately valid in the continuum limit. From these approximate expressions we find no extended states for the energies not equal to the onsite energy in the continuum limit in agreement with our scaling argument.

The techniques developed are general and can be applied to related systems such as the random Schrödinger equation and disordered Kronig-Penney-type models in which transport properties can be studied. Recently, extended states in Thue-Morse chains have been found and has led to a new type of correlated disorder.[8,9] The techniques developed can be applied to such systems and may provide valuable insight into the nature of this new type of correlated disorder.

ACKNOWLEDGMENT

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APPENDIX: PARAMETRIZATION OF THE CONFORMAL MAP

It is convenient to rescale the mapping by defining $v_n = r_n e^{-i\theta_n}$, where $\theta_n = \tan^{-1}[2V/(E-\epsilon_n)]$. The map can be parametrized by $v_n = \coth(\zeta_n)$ and $|z_n| = \coth(\phi_n)$. The parametrized map is given by

$$\coth(\zeta_{n+1}) = e^{-i(\theta_n+\theta_{n+1})}\coth(\zeta_n+\phi_n), \tag{A1}$$

and in terms of the parametrized map we obtain

$$\Lambda_N^{(+)}(E) = \prod_{n=1}^{N}\left(\frac{E-\epsilon_n}{2V}\right)e^{i\theta_n}\left(\frac{\sinh(\zeta_n+\phi_n)}{\sinh(\zeta_n)\sinh(\phi_n)}\right). \tag{A2}$$

The Lyapunov exponent in terms of the parametrized map is given by

$$\gamma_N(E) = \frac{1}{N}\sum_{n=1}^{N}\left[\ln\left(\frac{E-\epsilon_n}{2V}\right)+i\theta_n\right]+\overline{\gamma}, \tag{A3}$$

where

$$\overline{\gamma} = \frac{1}{N}\sum_{n=1}^{N}\ln\left(\frac{\sinh(\zeta_n+\phi_n)}{\sinh(\zeta_n)\sinh(\phi_n)}\right). \tag{A4}$$

The Lyapunov exponent is a complex-valued quantity in which the real part is the inverse of the localization length and the imaginary part is the integrated density of states.

From the numerical results on the iterated conformal map given in Eq. (12) we obtain the approximate convergence $r_n \approx e^{i\theta_n+i\delta_n}$. From the approximate expression it is possible to derive a phase map for δ_n given by

$$\delta_{n+1} = \delta_n - (\theta_{n+1}+\theta_n) + 2\sum_{k=1}^{\infty}\frac{(-)^k}{k}\left(\frac{\sin(k\delta_n)}{|z_n|^k}\right), \tag{A5}$$

where we have made use of $1 < |z_n|$. Neglecting the terms of order $(1/|z_n|)$ and higher, we obtain the approximate phase map used in Sec. IV.

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